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Erratum: "Assessment of interaction-strength interpolation formulas for gold and silver clusters" [J. Chem. Phys. 148, 134106 (2018)]

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With this Erratum, we provide corrections to certain mistakes appearing in the original publication.[1]

Namely, in Eq. (12), the λ-dependent Hamiltonian for the Hartree-Fock adiabatic connection lacks the external potential term. The correct equation is

$$\hat{H}^{\lambda} = \hat{T} + \hat{V}_{\mathrm{HF}} + \hat{V}_{\mathrm{ext}} + \lambda\,(\hat{V}_{ee} - \hat{V}_{\mathrm{HF}}). \tag{1}$$

The typos listed in the following all appear in the appendix. The parameter c in Eq. (A6) is wrong by a factor of two; the correct expression reads as follows:

$$c = \frac{4(W_0' W_\infty')^2}{(W_0 - W_\infty)^4}. \tag{2}$$

In Eq. (A13), we have incorrectly used the parameter "c"; "c" has to be replaced by "γ," as defined in Eq. (A12). Also, the expression lacks the exchange energy. Thus, the proper expression reads as follows:

$$E_{xc}^{\mathrm{LB}} = 2\beta\left[\frac{1}{\gamma}\left(\sqrt{1+\gamma} - \frac{1+\gamma/2}{1+\gamma}\right) - 1\right] + W_0. \tag{3}$$

Finally, in Eqs. (A14) and (A15), the fractional powers appearing in the first terms are powers of the density and not of the position vector. Hence,

$$W_\infty \approx W_\infty^{\mathrm{PC}} = \int\left[A\rho^{4/3}(\mathbf{r}) + B\frac{|\nabla\rho(\mathbf{r})|^2}{\rho^{4/3}(\mathbf{r})}\right]d\mathbf{r}, \tag{4}$$

$$W_\infty' \approx W_\infty'^{\,\mathrm{PC}} = \int\left[C\rho^{3/2}(\mathbf{r}) + D\frac{|\nabla\rho(\mathbf{r})|^2}{\rho^{7/6}(\mathbf{r})}\right]d\mathbf{r}. \tag{5}$$

These corrections do not alter any of the results or conclusions shown in the paper.

[1]S. Giarrusso, P. Gori-Giorgi, F. Della Sala, and E. Fabiano, J. Chem. Phys. **148**, 134106 (2018).